Safety data sheet

acc. to Safe Work Australia - Code of Practice

Benzoic acid benzyl ester ≥99 %, for synthesis

article number: **9498**
Version: **GHS 4.0 en**
Replaces version of: 2022-04-01
Version: (GHS 3)

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Revision: 2024-03-02

SECTION 1: Identification of the substance/mixture and of the company/ undertaking

1.1 Product identifier

Identification of the substance	**Benzoic acid benzyl ester** ≥99 %, for synthesis
Article number	9498
CAS number	120-51-4
Alternative name(s)	Benzyl benzoate

1.2 Relevant identified uses of the substance or mixture and uses advised against

Relevant identified uses:	Laboratory chemical Laboratory and analytical use
Uses advised against:	Do not use for private purposes (household). Food, drink and animal feedingstuffs.

1.3 Details of the supplier of the safety data sheet

Carl Roth GmbH + Co. KG
Schoemperlenstr. 3-5
D-76185 Karlsruhe
Germany

Telephone:+49 (0) 721 - 56 06 0
Telefax: +49 (0) 721 - 56 06 149
e-mail: sicherheit@carlroth.de
Website: www.carlroth.de

Competent person responsible for the safety data sheet:	Department Health, Safety and Environment
e-mail (competent person):	**sicherheit@carlroth.de**

1.4 Emergency telephone number

Name	Street	Postal code/city	Telephone	Website
NSW Poisons Information Centre Childrens Hospital	Hawkesbury Road	2145 West-mead, NSW	131126	

SECTION 2: Hazards identification

2.1 Classification of the substance or mixture

Classification acc. to GHS

Section	Hazard class	Cat-egory	Hazard class and category	Hazard statement
3.1O	Acute toxicity (oral)	4	Acute Tox. 4	H302

For full text of abbreviations: see SECTION 16

2.2 Label elements

Labelling

Signal word **Warning**

Pictograms

GHS07

Hazard statements

H302 Harmful if swallowed

Precautionary statements

Precautionary statements - prevention

P264 Wash thoroughly after handling
P270 Do not eat, drink or smoke when using this product

Precautionary statements - response

P301+P312 IF SWALLOWED: Call a POISON CENTER or doctor/physician if you feel unwell
P330 Rinse mouth

Precautionary statements - disposal

P501 Dispose of contents/container to industrial combustion plant

2.3 Other hazards

Results of PBT and vPvB assessment

According to the results of its assessment, this substance is not a PBT or a vPvB.

Endocrine disrupting properties

Does not contain an endocrine disruptor (ED) at a concentration of ≥ 0,1%.

SECTION 3: Composition/information on ingredients

3.1 Substances

Name of substance	Benzoic acid benzyl ester
Molecular formula	$C_{14}H_{12}O_2$
Molar mass	213.3 $^{g}/_{mol}$
CAS No	120-51-4

SECTION 4: First aid measures

4.1 Description of first aid measures

General notes

Take off contaminated clothing.

Following inhalation

Provide fresh air. In all cases of doubt, or when symptoms persist, seek medical advice.

Following skin contact

Rinse skin with water/shower. In all cases of doubt, or when symptoms persist, seek medical advice.

Following eye contact

Rinse cautiously with water for several minutes. In all cases of doubt, or when symptoms persist, seek medical advice.

Following ingestion

Rinse mouth with water (only if the person is conscious). Call a doctor.

4.2 Most important symptoms and effects, both acute and delayed

Irritant effects, Nausea, Vomiting, Spasms, Loss of righting reflex, and ataxia

4.3 Indication of any immediate medical attention and special treatment needed

none

SECTION 5: Firefighting measures

5.1 Extinguishing media

Suitable extinguishing media

co-ordinate firefighting measures to the fire surroundings!
water spray, dry extinguishing powder, BC-powder, carbon dioxide (CO_2)

Unsuitable extinguishing media

water jet

5.2 Special hazards arising from the substance or mixture

Combustible. Vapours are heavier than air, spread along floors and form explosive mixtures with air.

Hazardous combustion products

In case of fire may be liberated: Carbon monoxide (CO), Carbon dioxide (CO_2)

5.3 Advice for firefighters

In case of fire and/or explosion do not breathe fumes. Fight fire with normal precautions from a reasonable distance. Wear self-contained breathing apparatus.

SECTION 6: Accidental release measures

6.1 Personal precautions, protective equipment and emergency procedures

For non-emergency personnel

Avoid contact with skin, eyes and clothes. Do not breathe vapour/spray.

6.2 Environmental precautions

Keep away from drains, surface and ground water. Retain contaminated washing water and dispose of it. If substance has entered a water course or sewer, inform the responsible authority.

6.3 Methods and material for containment and cleaning up

Advice on how to contain a spill

Covering of drains.

Advice on how to clean up a spill

Absorb with liquid-binding material (sand, diatomaceous earth, acid- or universal binding agents).

Other information relating to spills and releases

Place in appropriate containers for disposal. Ventilate affected area.

6.4 Reference to other sections

Hazardous combustion products: see section 5. Personal protective equipment: see section 8. Incompatible materials: see section 10. Disposal considerations: see section 13.

SECTION 7: Handling and storage

7.1 Precautions for safe handling

Provision of sufficient ventilation.

Advice on general occupational hygiene

Wash hands before breaks and after work. Keep away from food, drink and animal feedingstuffs.

7.2 Conditions for safe storage, including any incompatibilities

Keep container tightly closed.

Incompatible substances or mixtures

Observe hints for combined storage.

Consideration of other advice:

Specific designs for storage rooms or vessels

Recommended storage temperature: 15 – 25 °C

7.3 Specific end use(s)

No information available.

SECTION 8: Exposure controls/personal protection

8.1 Control parameters

National limit values

Occupational exposure limit values (Workplace Exposure Limits)

This information is not available.

Human health values

Relevant DNELs and other threshold levels

Endpoint	Threshold level	Protection goal, route of exposure	Used in	Exposure time
DNEL	5.1 mg/m³	human, inhalatory	worker (industry)	chronic - systemic effects
DNEL	102 mg/m³	human, inhalatory	worker (industry)	acute - systemic effects

Relevant DNELs and other threshold levels				
Endpoint	**Threshold level**	**Protection goal, route of exposure**	**Used in**	**Exposure time**
DNEL	2.6 mg/kg bw/ day	human, dermal	worker (industry)	chronic - systemic effects

Environmental values

Relevant PNECs and other threshold levels				
End-point	**Threshold level**	**Organism**	**Environmental com-partment**	**Exposure time**
PNEC	0.017 $^{mg}/_{l}$	aquatic organisms	freshwater	short-term (single instance)
PNEC	0.002 $^{mg}/_{l}$	aquatic organisms	marine water	short-term (single instance)
PNEC	100 $^{mg}/_{l}$	aquatic organisms	sewage treatment plant (STP)	short-term (single instance)
PNEC	10.66 $^{mg}/_{kg}$	aquatic organisms	freshwater sediment	short-term (single instance)
PNEC	1.07 $^{mg}/_{kg}$	aquatic organisms	marine sediment	short-term (single instance)
PNEC	2.12 $^{mg}/_{kg}$	terrestrial organisms	soil	short-term (single instance)

8.2 Exposure controls

Individual protection measures (personal protective equipment)

Eye/face protection

Use safety goggle with side protection.

Skin protection

• hand protection

Wear suitable gloves. Chemical protection gloves are suitable, which are tested according to EN 374. For special purposes, it is recommended to check the resistance to chemicals of the protective gloves mentioned above together with the supplier of these gloves. The times are approximate values from measurements at 22 ° C and permanent contact. Increased temperatures due to heated substances, body heat etc. and a reduction of the effective layer thickness by stretching can lead to a considerable reduction of the breakthrough time. If in doubt, contact manufacturer. At an approx. 1.5 times larger / smaller layer thickness, the respective breakthrough time is doubled / halved. The data apply only to the pure substance. When transferred to substance mixtures, they may only be considered as a guide.

• type of material

Butyl caoutchouc (butyl rubber)

• material thickness

0,5 mm

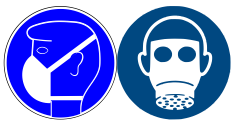
• breakthrough times of the glove material

>480 minutes (permeation: level 6)

• other protection measures

Take recovery periods for skin regeneration. Preventive skin protection (barrier creams/ointments) is recommended.

Respiratory protection



Respiratory protection necessary at: Aerosol or mist formation. Type: A (against organic gases and vapours with a boiling point of > 65 °C , colour code: Brown).

Environmental exposure controls

Keep away from drains, surface and ground water.

SECTION 9: Physical and chemical properties

9.1 Information on basic physical and chemical properties

Physical state	liquid
Colour	colourless
Odour	characteristic
Melting point/freezing point	21 °C (ECHA)
Boiling point or initial boiling point and boiling range	323 – 324 °C
Flammability	this material is combustible, but will not ignite readily
Lower and upper explosion limit	not determined
Flash point	148 °C at 101.3 kPa (ECHA)
Auto-ignition temperature	480 °C (ECHA)
Decomposition temperature	not relevant
pH (value)	not determined
Kinematic viscosity	not determined
Dynamic viscosity	10.9 mPa s at 25 °C
Solubility(ies)	
Water solubility	(poorly soluble)
Partition coefficient	
Partition coefficient n-octanol/water (log value):	3.97 (25 °C) (ECHA)
Soil organic carbon/water (log KOC)	3.8 (ECHA)
Vapour pressure	<0.1 hPa at 20 °C

Density and/or relative density	
Density	1.12 $^{g}/_{cm^3}$ at 20 °C
Relative vapour density	7.31 (air = 1)
Particle characteristics	not relevant (liquid)
Other safety parameters	
Oxidising properties	none

9.2 Other information

Information with regard to physical hazard classes:	hazard classes acc. to GHS (physical hazards): not relevant
Other safety characteristics:	There is no additional information.

SECTION 10: Stability and reactivity

10.1 Reactivity

This material is not reactive under normal ambient conditions.

If heated

Vapours may form explosive mixtures with air.

10.2 Chemical stability

The material is stable under normal ambient and anticipated storage and handling conditions of temperature and pressure.

10.3 Possibility of hazardous reactions

Violent reaction with: strong oxidiser

10.4 Conditions to avoid

Keep away from heat.

10.5 Incompatible materials

different plastics, Light metals

10.6 Hazardous decomposition products

Hazardous combustion products: see section 5.

SECTION 11: Toxicological information

11.1 Information on toxicological effects

Classification acc. to GHS

Acute toxicity

Harmful if swallowed.

Acute toxicity

Exposure route	Endpoint	Value	Species	Method	Source
oral	LD50	>2,000 $^{mg}/_{kg}$	rat		ECHA

Skin corrosion/irritation

Shall not be classified as corrosive/irritant to skin.

Serious eye damage/eye irritation

Shall not be classified as seriously damaging to the eye or eye irritant.

Respiratory or skin sensitisation

Shall not be classified as a respiratory or skin sensitiser.

Germ cell mutagenicity

Shall not be classified as germ cell mutagenic.

Carcinogenicity

Shall not be classified as carcinogenic.

Reproductive toxicity

Shall not be classified as a reproductive toxicant.

Specific target organ toxicity - single exposure

Shall not be classified as a specific target organ toxicant (single exposure).

Specific target organ toxicity - repeated exposure

Shall not be classified as a specific target organ toxicant (repeated exposure).

Aspiration hazard

Shall not be classified as presenting an aspiration hazard.

Symptoms related to the physical, chemical and toxicological characteristics

• If swallowed

vomiting, nausea, Spasms, gastrointestinal complaints, loss of righting reflex, and ataxia

• If in eyes

slightly irritant but not relevant for classification

• If inhaled

irritant effects

• If on skin

Frequently or prolonged contact with skin may cause dermal irritation

• Other information

none

11.2 Endocrine disrupting properties

Does not contain an endocrine disruptor (ED) at a concentration of ≥ 0,1%.

SECTION 12: Ecological information

12.1 Toxicity

Very toxic to aquatic life with long lasting effects.

Aquatic toxicity (acute)				
Endpoint	**Value**	**Species**	**Source**	**Exposure time**
LC50	0.29 $^{mg}/_{l}$	striped brill		96 h
EC50	3.09 $^{mg}/_{l}$	aquatic invertebrates	ECHA	48 h
ErC50	0.475 $^{mg}/_{l}$	algae	ECHA	72 h

Aquatic toxicity (chronic)				
Endpoint	**Value**	**Species**	**Source**	**Exposure time**
LC50	11 $^{mg}/_{l}$	aquatic invertebrates	ECHA	24 h
EC50	>10,000 $^{mg}/_{l}$	microorganisms	ECHA	3 h

12.2 Persistence and degradability

Theoretical Oxygen Demand: 2.401 $^{mg}/_{mg}$
Theoretical Carbon Dioxide: 2.889 $^{mg}/_{mg}$

Biodegradation

The substance is readily biodegradable.

Process of degradability		
Process	**Degradation rate**	**Time**
biotic/abiotic	94 %	28 d
oxygen depletion	94 %	28 d

12.3 Bioaccumulative potential

Does not significantly accumulate in organisms.

n-octanol/water (log KOW)	3.97 (25 °C) (ECHA)
BCF	193.4 (ECHA)

12.4 Mobility in soil

The Organic Carbon normalised adsorption coefficient	3.8 (ECHA)

12.5 Results of PBT and vPvB assessment

According to the results of its assessment, this substance is not a PBT or a vPvB.

12.6 Endocrine disrupting properties

Does not contain an endocrine disruptor (ED) at a concentration of ≥ 0,1%.

12.7 Other adverse effects

Data are not available.

SECTION 13: Disposal considerations

13.1 Waste treatment methods

This material and its container must be disposed of as hazardous waste. Dispose of contents/container in accordance with local/regional/national/international regulations.

Sewage disposal-relevant information

Do not empty into drains.

Waste treatment of containers/packagings

Only packagings which are approved (e.g. acc. to the Dangerous Goods Regulations) may be used. Handle contaminated packages in the same way as the substance itself. Completely emptied packages can be recycled.

13.3 Remarks

Waste shall be separated into the categories that can be handled separately by the local or national waste management facilities. Please consider the relevant national or regional provisions. Non-contaminated packages may be recycled.

SECTION 14: Transport information

14.1 UN number

UN RTDG	UN 3082
IMDG-Code	UN 3082
ICAO-TI	UN 3082

14.2 UN proper shipping name

UN RTDG	ENVIRONMENTALLY HAZARDOUS SUBSTANCE, LIQUID, N.O.S.
IMDG-Code	ENVIRONMENTALLY HAZARDOUS SUBSTANCE, LIQUID, N.O.S.
ICAO-TI	Environmentally hazardous substance, liquid, n.o.s.
Technical name	Benzoic acid benzyl ester

14.3 Transport hazard class(es)

UN RTDG	9
IMDG-Code	9
ICAO-TI	9

14.4 Packing group

UN RTDG	III
IMDG-Code	III
ICAO-TI	III

14.5 Environmental hazards

hazardous to the aquatic environment

14.6 Special precautions for user

There is no additional information.

14.7 Transport in bulk according to IMO instruments

The cargo is not intended to be carried in bulk.

14.8 Information for each of the UN Model Regulations

Transport informationNational regulationsAdditional information(UN RTDG)	
UN number	3082
Class	9
Environmental hazards	Yes Hazardous to the aquatic environment
Packing group	III
Danger label(s)	9 Fish and tree

Special provisions (SP)	274, 331, 335, 375 UN RTDG
Excepted quantities (EQ)	E1 UN RTDG
Limited quantities (LQ)	5 L UN RTDG
Emergency Action Code	3Z

International Maritime Dangerous Goods Code (IMDG) - Additional information

Proper shipping name	ENVIRONMENTALLY HAZARDOUS SUBSTANCE, LIQUID, N.O.S.
Particulars in the shipper's declaration	UN3082, ENVIRONMENTALLY HAZARDOUS SUBSTANCE, LIQUID, N.O.S., (Benzoic acid benzyl ester), 9, III
Marine pollutant	yes (hazardous to the aquatic environment), (Benzoic acid benzyl ester)
Danger label(s)	9, "Fish and tree"

Special provisions (SP)	274, 335, 969
Excepted quantities (EQ)	E1
Limited quantities (LQ)	5 L
EmS	F-A, S-F
Stowage category	A

International Civil Aviation Organization (ICAO-IATA/DGR) - Additional information

Proper shipping name	Environmentally hazardous substance, liquid, n.o.s.
Particulars in the shipper's declaration	UN3082, Environmentally hazardous substance, liquid, n.o.s., (Benzoic acid benzyl ester), 9, III
Environmental hazards	yes (hazardous to the aquatic environment)
Danger label(s)	9, "Fish and tree"

Special provisions (SP)	A97, A158, A197, A215
Excepted quantities (EQ)	E1
Limited quantities (LQ)	30 kg

SECTION 15: Regulatory information

15.1 Safety, health and environmental regulations/legislation specific for the substance or mixture

There is no additional information.

National regulations(Australia)

Australian Inventory of Chemical Substances(AICS)

Substance is listed.

Other information

Directive 94/33/EC on the protection of young people at work. Observe employment restrictions under the Maternity Protection Directive (92/85/EEC) for expectant or nursing mothers.

National inventories

Country	Inventory	Status
AU	AIIC	substance is listed
CA	DSL	substance is listed
CN	IECSC	substance is listed
EU	ECSI	substance is listed
EU	REACH Reg.	substance is listed
JP	CSCL-ENCS	substance is listed
JP	ISHA-ENCS	substance is listed
KR	KECI	substance is listed
MX	INSQ	substance is listed
NZ	NZIoC	substance is listed
PH	PICCS	substance is listed
TR	CICR	substance is listed
TW	TCSI	substance is listed
US	TSCA	substance is listed (ACTIVE)

Country	Inventory	Status
VN	NCI	substance is listed

Legend

AIIC	Australian Inventory of Industrial Chemicals
CICR	Chemical Inventory and Control Regulation
CSCL-ENCS	List of Existing and New Chemical Substances (CSCL-ENCS)
DSL	Domestic Substances List (DSL)
ECSI	EC Substance Inventory (EINECS, ELINCS, NLP)
IECSC	Inventory of Existing Chemical Substances Produced or Imported in China
INSQ	National Inventory of Chemical Substances
ISHA-ENCS	Inventory of Existing and New Chemical Substances (ISHA-ENCS)
KECI	Korea Existing Chemicals Inventory
NCI	National Chemical Inventory
NZIoC	New Zealand Inventory of Chemicals
PICCS	Philippine Inventory of Chemicals and Chemical Substances (PICCS)
REACH Reg.	REACH registered substances
TCSI	Taiwan Chemical Substance Inventory
TSCA	Toxic Substance Control Act

15.2 Chemical Safety Assessment

No Chemical Safety Assessment has been carried out for this substance.

SECTION 16: Other information

Indication of changes (revised safety data sheet)

Section	Former entry (text/value)	Actual entry (text/value)	Safety-relevant
2.3		Endocrine disrupting properties: Does not contain an endocrine disruptor (ED) at a concentration of ≥ 0,1%.	yes
14.8		Emergency Action Code: 3Z	yes
15.1		National inventories: change in the listing (table)	yes

Abbreviations and acronyms

Abbr.	Descriptions of used abbreviations
BCF	Bioconcentration factor
CAS	Chemical Abstracts Service (service that maintains the most comprehensive list of chemical substances)
DGR	Dangerous Goods Regulations (see IATA/DGR)
DNEL	Derived No-Effect Level
EC50	Effective Concentration 50 %. The EC50 corresponds to the concentration of a tested substance causing 50 % changes in response (e.g. on growth) during a specified time interval
ED	Endocrine disruptor
EINECS	European Inventory of Existing Commercial Chemical Substances
ELINCS	European List of Notified Chemical Substances
EmS	Emergency Schedule
ErC50	≡ EC50: in this method, that concentration of test substance which results in a 50 % reduction in either growth (EbC50) or growth rate (ErC50) relative to the control
GHS	"Globally Harmonized System of Classification and Labelling of Chemicals" developed by the United Nations

Abbr.	Descriptions of used abbreviations
IATA	International Air Transport Association
IATA/DGR	Dangerous Goods Regulations (DGR) for the air transport (IATA)
ICAO	International Civil Aviation Organization
ICAO-TI	Technical instructions for the safe transport of dangerous goods by air
IMDG	International Maritime Dangerous Goods Code
IMDG-Code	International Maritime Dangerous Goods Code
LC50	Lethal Concentration 50%: the LC50 corresponds to the concentration of a tested substance causing 50 % lethality during a specified time interval
LD50	Lethal Dose 50 %: the LD50 corresponds to the dose of a tested substance causing 50 % lethality during a specified time interval
NLP	No-Longer Polymer
PBT	Persistent, Bioaccumulative and Toxic
PNEC	Predicted No-Effect Concentration
UN RTDG	UN Recommendations on the Transport of Dangerous Good
vPvB	Very Persistent and very Bioaccumulative

Key literature references and sources for data

Safe Work Australia's Code of Practice for Labelling of Workplace Hazardous Chemicals (under WHS Regulations).

UN Recommendations on the Transport of Dangerous Good. International Maritime Dangerous Goods Code (IMDG). Dangerous Goods Regulations (DGR) for the air transport (IATA).

List of relevant phrases (code and full text as stated in section 2 and 3)

Code	Text
H302	Harmful if swallowed.

Disclaimer

This information is based upon the present state of our knowledge. This SDS has been compiled and is solely intended for this product.